An Improved Analytic Technique to Predict Space System Contamination

By

R. R. Hale

Aerojet ElectroSystems Company
Azusa, California

A new mathematical model to predict diffusion mass transport among surfaces is described which accounts for inter-molecular collisional behavior. The mathematical characterization utilizes dynamic thermal history behavior for the surfaces of interest. It evaluates the instantaneous local atmospheric pressure prior to and during ascent to calculate molecular collision probabilities. Adsorption coefficients for various temperatures are evaluated for each surface in a manner which simulates their mission temperature cycles. The input data for this portion of the contamination model is developed from thermal models, and a "sojourn" time and accommodation coefficient description is applied to surface behavior.

The model has been used to predict net contamination conditions at insertion for a geosynchronous satellite launched on a Titan 34D vehicle. Output data from that analysis is presented and further applications to alternative launch techniques are reviewed. A description of the parametric index which allows selection of either the diffusion or the line-of-sight contamination transport calculations, as appropriate to the mission instantaneous environment, is also given.

1.0 INTRODUCTION

In the analysis and mathematical characterization of contamination processes related to space missions, two separate mass transport regimes can be defined. Heretofore, the more widely investigated of these two regimes has been line-of-sight behavior in which molecules or particles can travel over significant distances before colliding with other bodies. This condition prevails in deep space and is characterized by relatively low population densities of molecular species in the local environment. Typical molecular concentrations, for example, are in the order of 10^{10} molecules per cubic centimeter or less. The corresponding mean free path is of the order 10^4 centimeters (10^2 meters) or longer. Such conditions characterize the orbital environment of most spacecraft with reasonable accuracy. Under these "line-of-sight" transport conditions, it is convenient to express the mass transport behavior of materials in terms of a "view-factor" analysis which describes the geometric relationships of source and target pairs. The view factor contamination prediction is valid if one assumes that external forces acting on the molecules or particles are negligibly small, that intermediate collisions essentially do not occur, and that the source material particles are emitted with a mathematically defined directional characteristic. (Possible forces include electrostatic, magnetic, and gravitational ones.) Other investigators have reviewed spacecraft contamination behavior under "line-of-sight" assumptions with various degrees of rigor in recent literature.

The mass transport ("contamination") behavior which occurs prior to insertion of the spacecraft in deep space vacuum, however, has not been prominently treated in the literature. The essential difference is that a nonnegligible probability of interactions, or collisions, exists due to the higher concentration of ambient molecules. At normal atmospheric pressure, for example, the molecular concentration is

of the order 10^{19} molecules per cubic centimeter. The corresponding mean free path is less than 10^{-5} centimeters (10^{-7} meters). The effect of repetitive collisions is to randomize the direction of molecule (particle) motion, thereby giving rise to gaseous diffusion mass transport which is omnidirectional. In addition, since this diffusion transport behavior is not restricted to straight line travel, it is not subject to shadowing influences. Therefore, material transport by diffusion departs significantly from line-of-sight concepts and effects. This transport mode requires, then, a different mathematical and conceptual approach for application to pre-orbital spacecraft contamination studies. The value of such an analytical tool for space vehicles which are increasingly contaminant-sensitive, particularly for long-lived missions, appears to warrant developmental effort. This paper summarizes the results of Aerojet's recent activities in the mathematical and computer modeling of gaseous diffusion-transport contamination, and reviews a simple preliminary model which was applied to a particular launch and ascent sequence for a geosynchronous satellite mission.

2.0 BACKGROUND AND DEFINITIONS

In the field of space system contamination, mass transport can be characterized in three distinct modes.

2.1 Mode 1: Diffusion mass transport, typified by highly populous ambient molecules, generally gaseous. An example is the redistribution of material caused by molecular concentration gradients with respect to both time and distance.

2.2 Mode 2: Line-of-sight mass transport, characterized by the relative absence of ambient intermolecular collisions. An example is "backstreaming"

of pump fluids under certain conditions
in vacuum pumping.

2.3 Transition and Special Effects Modes: Mass transport
by mechanisms not described accurately by
either Mode 1 or Mode 2. Examples are
intermediate molecular concentration
regimes with combined viscous and non-
viscous flow, particulates, and active
forces, such as rocket exhausts, electro-
static and gravitational forces, and the
like.

This paper will address the Mode 1 mass transport only. It is
obviously appropriate to consider all three modes for total space sys-
tem contamination control. Figure 1 summarizes the approximate time
interval in a spacecraft's life cycle during which the respective con-
tamination transport mechanisms are active. The total life cycle time
during which contamination can occur begins with manufacture of the
space component or system and ends at the termination of its useful
life. Mode 1 contamination extends only through the launch and ascent
phases.

3.0 MATHEMATICAL APPROACH

The classical kinetic theory of gases is based on the assumptions
that matter is made up of molecules, and that the molecules have a
velocity which is related to the temperature of the gas. This yields
certain well-known mathematical relationships concerning the kinetic
energy of the various molecules. These values of kinetic energy
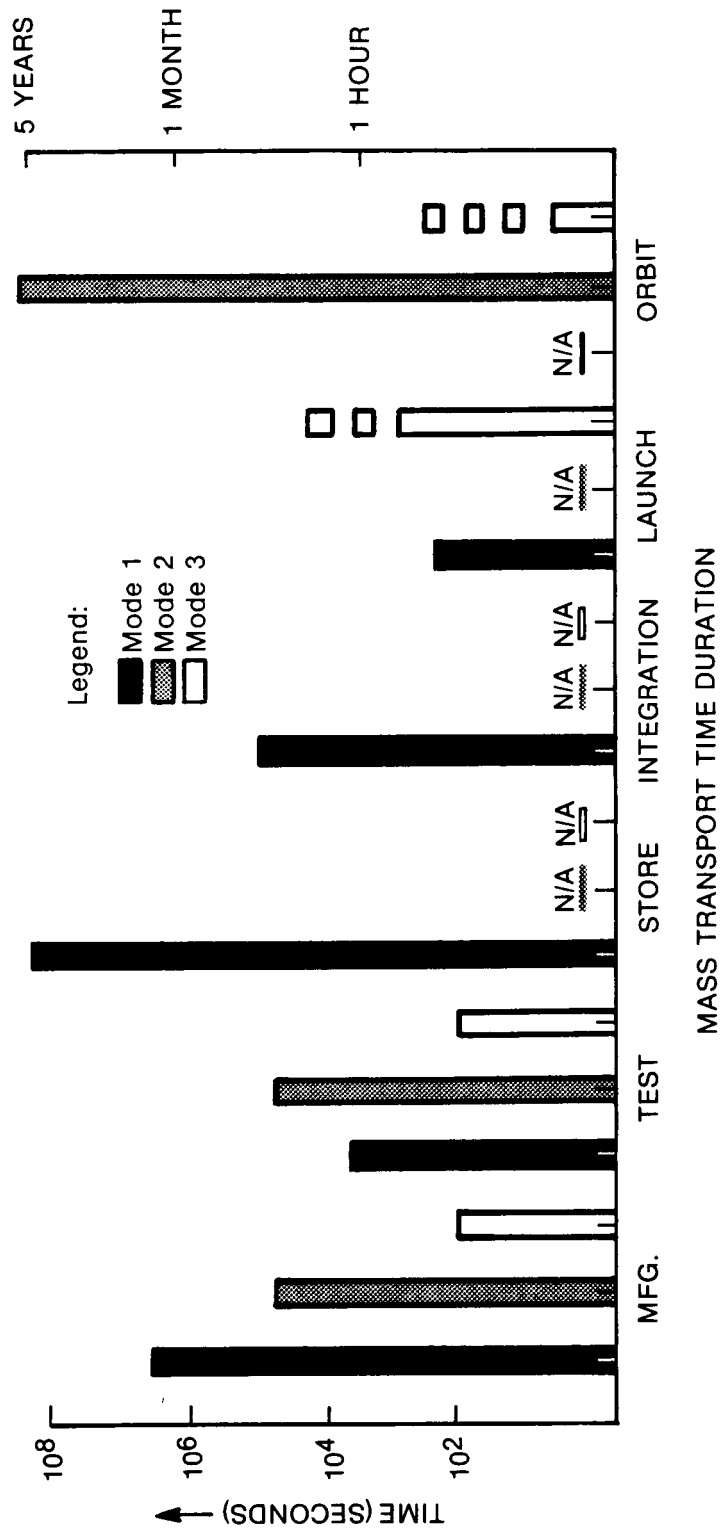depend on the molecular mass and on the velocity as:

Figure 1 Contamination modes and durations during spacecraft life cycle

$$E = \frac{1}{2} m_s v_s^2 \tag{1}$$

where

E is the translational kinetic energy

m_s is the mass for the characteristic molecular species

v_s is the velocity of the molecule

It was determined by Maxwell and Boltzman that a velocity distribution function could be expressed to characterize the range of variation of the molecular velocity. This is of the form:

$$\frac{1}{n}\frac{dn}{dv} = f_v = \frac{4}{\pi^{\frac{1}{2}}} \left(\frac{m}{2KT}\right)^{3/2} v^2 \exp\left(\frac{-mv^2}{2KT}\right) \tag{2}$$

where

f_v is the fractional number of molecules whose velocity ranges between v and (v + dv)

For this function, the value of f_v is zero for v = 0 and for v = ∞; f_v has its maximum value at:

$$v_p = (2KT/m)^{1/2}, \tag{3}$$

as can be seen by differentiating f_v with respect to v and setting the result equal to zero. V_p is the most probable velocity.

Application of Equation (2) to mathematically describe the properties of molecules in motion can yield different values of velocity, depending on the nature of the integration performed on the velocity distribution function. For example, if molecular kinetic energy

exchange is to be calculated, the significant term is the mean square of velocity, which yields

$$\bar{v}^2 = \int_0^\infty v^2 f_v \, dv \Big/ \int_0^\infty f_v \, dv = 3KT/m \tag{4}$$

from which, therefore,

$$v_2 = \left[\bar{v}_2\right]^{1/2} = (3KT/m)^{1/2} = 1.225 \, v_p \tag{5}$$

If, however, it is desired to evaluate bulk transport of gas, the appropriate velocity is

$$v_{avg} = \int_0^\infty v f_v \, dv \Big/ \int_0^\infty f_v \, dv = \frac{2}{\pi^{\frac{1}{2}}} (2KT/m)^{1/2} \tag{6}$$

therefore

$$v_{avg} = 1.128 \, v_p \tag{7}$$

It is erroneous to apply the value of Equation (3) indiscriminately in mathematical modeling work, and, moreover, it is preferable to express the velocity distribution and to perform integrations over the appropriate range of molecular velocities. Figure 2 illustrates the various values of velocity and the function of Equation (2). For net molecular transport, then Equation (6) will be used.

An extension of the classical kinetic theory which assumes perfectly elastic intermolecular and surface collisions gives rise to the so-called ideal gas relations. This is commonly expressed mathematically as
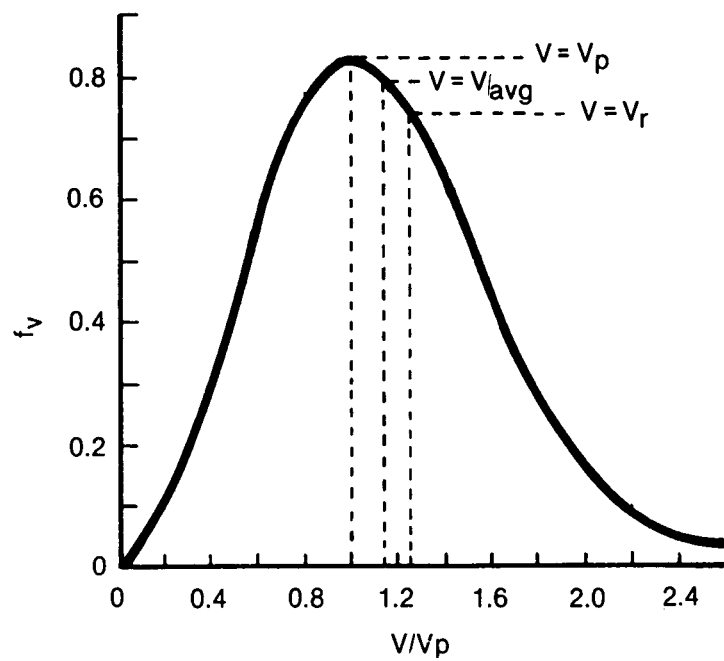
Figure 2 Maxwell-Boltzmann molecular velocity distribution function

$$PV = n R_O T \qquad (8)$$

where

P = the gas pressure

V = the volume occupied by the gas

n = the number of moles of gas in the volume V

R_O is a constant defined by the measurement system of units

T is the absolute temperature of the gas in the closed volume, V.

A simplifying assumption is made that the gases do not change state, making Van der Waals' correction terms unnecessary.

For the mathematical case of modeling an ideal closed system at equilibrium, the above expressions would apply. For the ascent transient analysis, however, three additional mathematical descriptors must be applied. The first of these is a characterization of the various physical surfaces to adsorb or desorb gas. A rigorous analysis of this complex behavior is beyond the scope of this paper. With simplifications, however, an approximation of this behavior can be described in the form [1]:

$$N_O \theta = 3.51 \times 10^{22} \left[P/MT \right]^{1/2} f\, t' \exp \left[E_D/R_O T_s \right] (1 - \theta) \qquad (9)$$

where

T is the temperature of the gas

T_s is the temperature of the surface

t' is the period of oscillation of the molecule normal to the surface (approximately 10^{-13} seconds)

E_D is the energy for desorption.

---

1. Roth, A., Vacuum Technology, North Holland Publishing Company, New York (1976), p. 175.

f is the sticking coefficient

P is the pressure

θ is the covered area, which is desorbing

$1-\theta$ is the uncovered area, which is adsorbing

N_o is the total number of molecules required to form one monolayer.

Equation (9) is only valid for less than a complete monolayer but
is used here due to its relative simplicity. More complex equations
can be used to describe the multilayer absorption case.

The second characteristic which must be described mathematically
is the "pump-down" of the payload compartment which results from the
reduction of local exterior atmospheric pressure with altitude. As the
launch vehicle ascends, gas outflow from its interior volumes occurs
in response to this pressure difference. Scialdone [2] has presented a
method for analytically evaluating internal chamber pressures, given
vent path parameters, outgassing characteristics of the spacecraft
materials, and the exterior pressure dynamic conditions. His compu-
tation method essentially requires simultaneous solution of flow equa-
tions, using parametric isothermal materials outgassing functions. In
a typical mission, the altitude-time interrelationship during ascent
will be predetermined by the launch vehicle and payload character-
istics. For example, typical time versus altitude characteristics are
indicated in Columns 1 and 2 of Table I. Handbook data [3] can readily
be used to establish the external pressure as a function of altitude.
This, in turn, provides a pressure versus time function, as illus-
trated by Columns 3 and 4 of Table I. Figure 3 graphically depicts

2. Scialdone, J. J., _Internal Pressures of a Spacecraft or Other
    System of Compartments, Connected in Various Ways and Including
    Outgassing Materials, in a Time-Varying Pressure Environment_,
    X-327-69-524, GSFC (1969).

3. U.S. Standard Atmosphere, 1976. NOAA, NASA, USAF. NOAA-S/T 76-
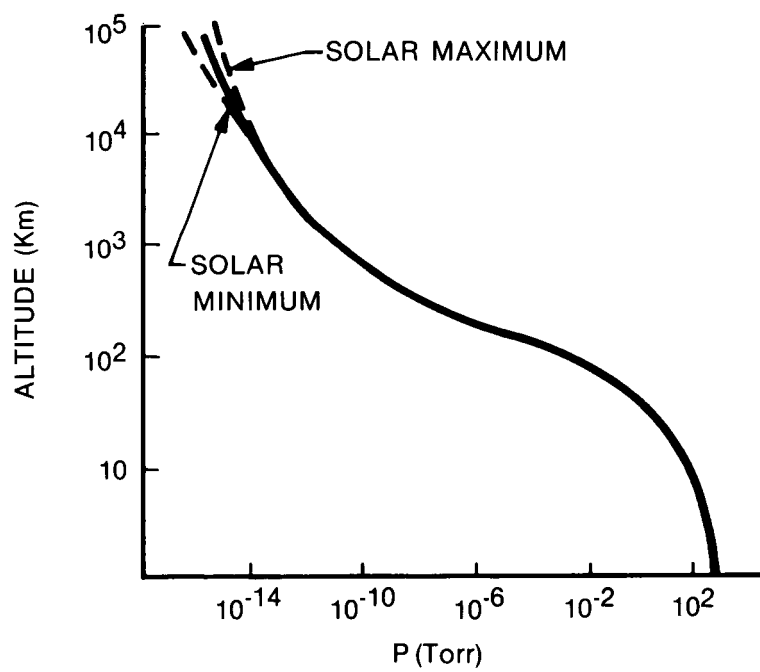   1562, USGPO, Washington, D.C., (1976).

Figure 3 Altitude - pressure relationship

the interrelationship of altitude and pressure. For this actual model analysis, the time increment resolution was taken arbitrarily as 10 seconds, rather than 50 as shown in the abbreviated table. Obviously, any appropriate time interval may be chosen, depending on the requirements of precision for the particular analytical model.

TABLE I

LAUNCH MISSION ALTITUDE AND PRESSURE DYNAMIC CHARACTERISTICS

Time from Launch (seconds)	Altitude (10^3 m)	Pressure (Torr)	Pressure (Pascal)
0	0	7.6×10^2	1.0×10^5
50	6.7	3.2×10^2	4.3×10^4
100	34	4.8	6.4×10^2
150	61	1.3×10^{-1}	1.7×10^1
200	87	2.3×10^{-3}	3.1×10^{-1}
250	110	5.3×10^{-5}	7.1×10^{-3}
300	131	8.8×10^{-6}	1.2×10^{-3}
350	144	4.5×10^{-6}	6.0×10^{-4}
400	151	3.3×10^{-6}	4.4×10^{-4}

The third dynamic characteristic which must be defined to apply this model is surface temperature behavior. Equation (9) requires the use of specific surface temperatures to evaluate the quasi-equilibrium adsorbed gas state. During the actual vehicle ascent, the surface temperatures are changing with time; in fact, various surfaces have different temperature change rates because of their thermal and mass properties and their design configuration interrelationships. Using a thermal model of the spacecraft, the effect of different payload fairing temperature histories on key contamination-sensitive surface temperatures was analytically investigated. For two such conditions,

241

which are characterized by the curves designated "maximum fairing temperature" and "minimum fairing temperature," the temperature of one thermal control surface can vary during ascent as shown in Figure 4. The curves indicate the predicted thermal control surface temperatures for "worst case" and "best case" payload fairing temperature conditions. The computed temperature difference is approximately 40 F degrees 300 seconds after launch. This results, of course, in significantly different desorption rates for the two launch cases. Further, it strongly suggests that some control is possible over launch phase intersurface mass transport by applying similar analyses and thermal design to optimize surface temperature histories.

A means for describing the net transport behavior of contaminant gases within the spacecraft environment is necessary. Whereas a net gas outflow occurs during ascent due to gross pressure changes as described above, gas composition gradients also change with time. The combination of theoretical energy and mass flux vector parameters and their driving forces are presented in Table II.

TABLE II

FORCES AND FLUXES (FROM IRREVERSIBLE THERMODYNAMICS)

Flux	Temperature Gradients	Composition Gradients, Pressure Gradients, Body Forces
Energy Flux, ϵ_i.	Fourier's Law	Diffusion thermo (Dufour effect)
Mass Flux j_{mi}.	Thermal Diffusion (Soret effect)	Fick's Law and extension

The energy flux caused by a composition gradient was discovered by Dufour in 1873; it is known as the Dufour effect and also as the diffusion-thermo effect. On the other hand, Soret established that
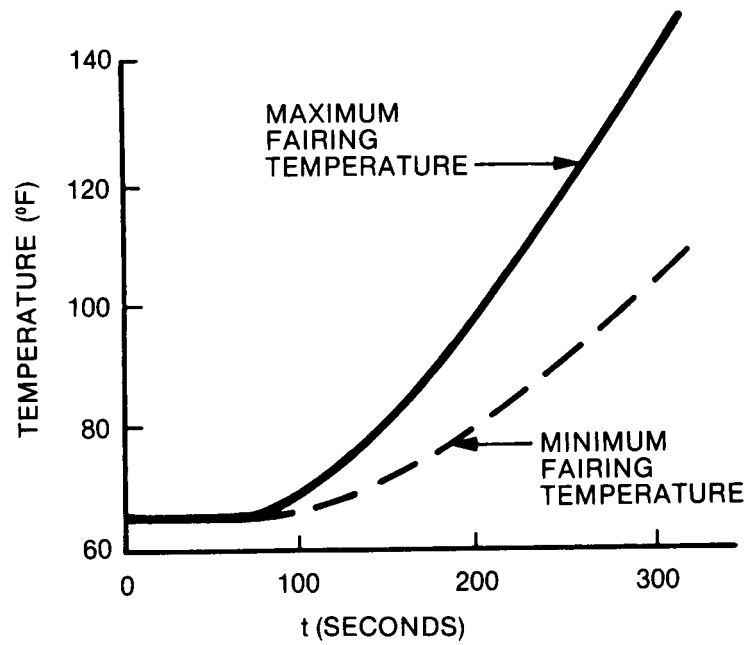
Figure 4   Predicted surface temperature vs.
time after launch

mass fluxes can also be created by temperature gradients. Since the thermal diffusion and diffusion-thermo effects are typically [4] of a smaller order of magnitude, they have been excluded for initial analytic work. The predominant force considered, then, is Fick's Law diffusion. With this condition, a material composition gradient causes mass transport in the direction of the lower concentration region. Fick's first law is expressed:

$$Q = -D_1 (dc/dx) \tag{10}$$

where

Q is the flow rate of diffusing gas
dc/dx is the concentration gradient
D_1 is the diffusion coefficient.

The negative sign describes the opposite flow direction with respect to the concentration gradient.

For cases in which equilibrium is reached only after long time periods or not at all, Fick's second law is also necessary.

$$D_1 \frac{d^2c}{dx^2} = \frac{dc}{dt} \tag{11}$$

Meyer [5] has established that, for two gases, the coefficient of interdiffusion is given by:

$$D_{12} = \frac{1}{3} \left[\lambda_1 V_{av_1} N_2 + \lambda_2 V_{av_2} N_1 \right] \Big/ (n_1 + n_2) \tag{12}$$

4. W. M. Kays, Convective Heat and Mass Transfer, McGraw Hill, N. Y. (1966).

5. Meyer, D. E., Journal of Vacuum Science and Technology, 11, 168 (1974).

For the situation in which the concentration of one of the gases is rather small, as is the case for contaminant vapors, then Equation (12) reduces to ⑥:

$$D_{12} = \frac{1}{3} \lambda_2 V_{av} = \frac{2}{3 \, \xi^2 \, P} \left(\frac{k^3 \, T^3}{\pi^3 \, m} \right)^{\frac{1}{2}} \tag{13}$$

in which

    m is the mass of the predominant molecule

    T is the temperature, °K

    k is Bolzmann's constant

    ξ is the molecular diameter

    P is the pressure.

An excellent literature review with tables of values for binary gas pair diffusion coefficients has been done by Marrero and Mason ⑦. The value for air-water at temperatures of concern in this analysis is 0.29 cm^2/s ⑧. For this simplified comparative modeling to date, the binary air-water gas system is assumed. The order of magnitude of displacements resulting from gaseous diffusion can be readily approximated. It was shown by Einstein that

$$\bar{X}^2 = 2 \, Dt \tag{14}$$

where:

    $\bar{X}$ is the distance executed by a particle

    t is the time duration

    D is the diffusion coefficient of the medium.

6. Roth, A., Vacuum Technology, North Holland Publishing Company, New York (1976).

7. Marrero, T. R., and Mason, E. A., J. Phys. Chem. Ref. Data, 1:3-118 (1972).

8. Sherwood, Thomas K.; Pigford, Robert L.; and Wilke, Charles R., Mass Transfer, McGraw Hill, N. Y., p. 23 (1975).

Since the diffusion coefficient values are typically a few tenths cm^2 per second at normal temperatures and pressures, the displacement is in the order of 1 cm per second. For the D value of 0.29 and a time of one second, we have, from Equation (14),

$$\bar{x}^2 \ = \ 2\,(.29)(1)$$

from which

$$\bar{X} \ = \ 7.6 \text{ mm in one second.}$$

A parameter is necessary to define the limit case in which gaseous diffusion is no longer significant. This situation occurs when the local molecular concentrations become sufficiently low that line-of-sight transport behavior occurs; that is, the molecules impinge on surfaces without intermolecular collisions. Strictly speaking, there occurs a transition concentration range during which some molecules statistically do not experience molecular collisions and some do. Detailed treatment of this transition regime is somewhat complex and should be separately addressed. However, for practical spacecraft contamination modeling, it is obviously important to address Mode 2 mass transport as well as Mode 1. A convenient parameter which can be routinely calculated and used as the program control variable is the mean free path. The expression for mean free path follows from Equations (6) and (8); it is commonly expressed as

$$\lambda \ = \ 2.33 \text{ x } 10^{-20}\, \frac{T}{\xi^2 P} \quad \text{(centimeters)} \tag{15}$$

Since the transport distance of interest in contamination analysis is typically in the order of a meter (10^2 cm), a convenient limit value for λ is thereby defined. Then, for $\lambda \leq 10^2$ cm, Mode 1 diffusion transport is stated to occur. Conversely, for $\lambda > 10^2$ cm, line

of sight (Mode 2) mass transport is indicated. A parameter which is
interrelated with λ is also available. The molecular incidence rate
is the number of molecules striking a surface element per unit time,
which can be shown to be

$$\phi = 3.513 \times 10^{22} \left[P/(MT)^{1/2} \right] \text{ molecules}\!\!\Big/\!\!_{\text{cm}^2} \text{ s.} \tag{16}$$

The interrelationship of the values for ϕ and λ for air at 25°C is
shown in Figure 5.

Together with the mission ascent parameters, Equations (9), (10),
(11), (13), and (15) form the basis for an iterative calculation model
which describes the dynamic contamination transport behavior for the
physical spacecraft system. It is necessary, of course, to construct
a math model of the surfaces of interest, including their relative
areas and the separation distances for all surface pairs. However, it
is not necessary to establish "view factors," as would be done for
radiation heat transfer or Mode 2 modeling. Since this modeling work
is new, simplifications have been used initially. These include the
binary gas assumptions and only two interacting surfaces. Superposi-
tion can be used to extend the model to describe other contaminants;
this would involve separate analysis of individual contaminants, each
of which would form an air-contaminant binary gas pair. The matrices
and the computations become more complex when multiple surfaces are
analyzed, but this is not a formidable problem. A further refinement
of this model would substitute more complex adsorption-desorption
expressions [9] for Equation (9).

---

9. Redheed, P. A., Hobson, J. P., and Kornelson, E. V., The Physical
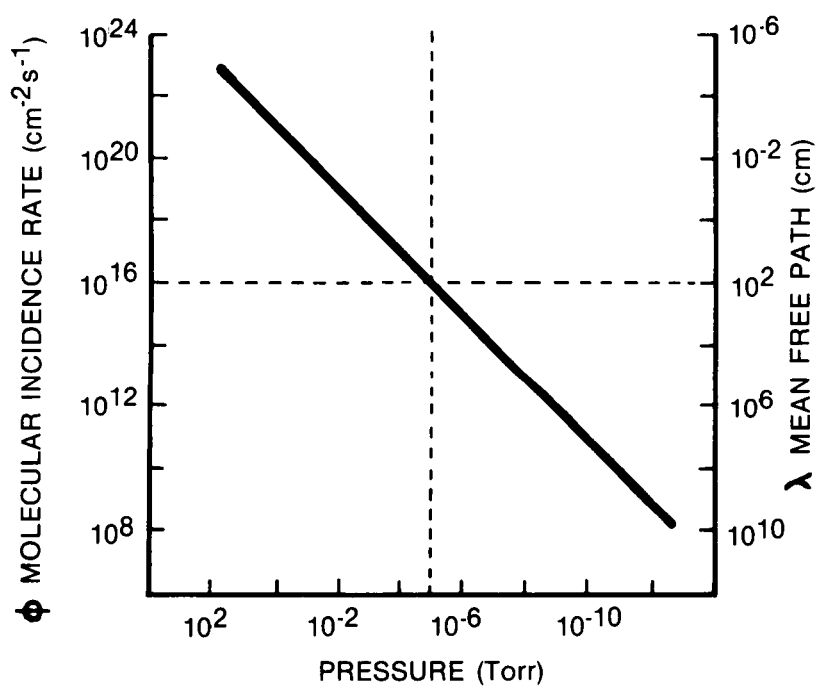   Basis of Ultra-High Vacuum, Chapman and Hall, London (1968).

Figure 5 λ and ϕ vs. pressure for air at 25ºC

4.0 APPLICATIONS

The model approach presented herein has a considerable amount of generality. Some analytic uses which suggest themselves include:

4.1 Prediction of contamination during storage.

4.2 "Self-contamination" analysis.

4.3 Contamination protection assessments.

4.4 Cyclic contamination evaluation (STS Orbiter).

4.5 Thermal-contamination interaction effects.

5.0 ACKNOWLEDGMENTS